

# Transport in quantum wells in the presence of interface roughness

Chung-Yu Mou<sup>(a)</sup> and Tzay-ming Hong<sup>(b)</sup>

*Department of Physics, National Tsing-Hua University, Hsinchu, Taiwan 30043,*

*Republic of China*

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## Abstract

The effective Hamiltonian for two dimensional quantum wells with rough interfaces is formally derived. Two new terms are generated. The first term is identified to the local energy level fluctuations, which was introduced phenomenologically in the literature for interface roughness scattering but is now shown to be valid only for an infinite potential well or Hamiltonians with one single length scale. The other term is shown to modulate the wavefunction and cause fluctuations in the charge density. This will further reduce the electron mobility to the magnitude that is close to the experimental result.

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## I. INTRODUCTION

The vast interest in the physics of charge transport in two-dimensional quantum wells stems from potential applications in new devices and subsequent integration with Si-based chip technology. Experimentally, it is known that the charge transport inside a quantum well is strongly affected by the quality of the well. In particular, it is believed that the interface roughness is inherent to the quantum well systems and plays an important role for wells at low temperature with small well widths<sup>1</sup>. On the theoretical side, starting from the seminar work by Kardar, Parisi, and Zhang<sup>2</sup>, a large effort has been devoted to understand the morphology of thin film growth<sup>3</sup> during the past decade. Nevertheless, these works only characterize long wavelength properties of the surface roughness, there is no systematic attempt to investigate how the electronic properties, such as the charge transport, are affected by the surface roughness.

The study of the effects of surface roughness on the electronic transport properties has a long history, tracing back to the work by Prange and Nee<sup>4</sup> on magnetic surface states in metals. Later, a more complete model was reconsidered by Ando<sup>5</sup>. Quite often, these works are summarized phenomenologically by introducing a local energy-level fluctuation term in potential:  $(\partial E/\partial L)\Delta(\mathbf{r})$ , where  $E$  is the energy eigenvalue of the electron,  $L$  is the averaged well width and  $\Delta(\mathbf{r})$  is the local change of quantum well width. Such phenomenology finds its natural application in interpreting the photoluminescence data of GaAs/AlAs quantum wells<sup>1,6</sup>. In this case, it has been established that for temperature less than 80 K, the linewidth of photoluminescence is mainly determined by the local energy level fluctuations. Transport properties of two-dimensional (2D) carrier gases at Si/SiO<sub>2</sub> interfaces and in semiconductor quantum wells are also shown to be strongly affected by the interface roughness<sup>7,8,10</sup>. In these studies, theoretical mobility is also calculated based on the assumption that the local energy level fluctuation is the dominant effect. It is known, however, that the experimentally observed mobility can not be explained solely by the roughness. In some parameter regime, one has to introduce, for example, phenomenologi-

cally negative impurity charge to account for the extra reduction of the mobility observed in experiments<sup>10,12</sup>.

In this work, we shall systematically investigate the effects of surface roughness. Our starting point is an averaged version of the Hamiltonian specialized to the quantum well configuration. In an expansion in  $\Delta(\mathbf{r})/L$ , two lowest order terms are considered. The first term is identified to the local energy level fluctuations  $(\partial E/\partial L)\Delta(\mathbf{r})$ . This term represents the mismatch effect of the energy band. It was introduced phenomenologically in the literature for interface roughness scattering, but is now shown to be valid only for an infinite potential well or Hamiltonians with one single length scale. The other term is shown to modulate the wavefunction and cause fluctuations in the charge density. This will further reduce the electron mobility.

The rest of the paper is organized as follows: In Section 2, we lay down the formulation of the effective Hamiltonian for two dimensional quantum wells. Some general features of the effective Hamiltonian are discussed. In particular, we expand the Hamiltonian to the order of  $\Delta(\mathbf{r})/L$  and discuss its effects on the basis of single particle states. In Section 3, we consider the fluctuation of the charge density caused by the wavefunction modulation, and study its consequence on the electron mobility to the order of  $\Delta(\mathbf{r})/L$ . In the final section, we examine the validity of our approach and conclude.

## II. THEORETICAL FORMULATION

Let us consider a generic quantum well specified by two interfaces at  $z = z_+(\mathbf{r})$  and  $z = z_-(\mathbf{r})$ , where  $\mathbf{r} = (x, y)$  is a two dimensional vector. The average distance between the two surfaces is  $L$  (see Fig.1). For simplicity, we shall impose the hard wall condition on the interfaces. Our formulation is easily generalized to the case when the potential well is finite. To investigate the effects that are due to the interface roughness, it is convenient to do a transformation that maps  $z_+(\mathbf{r})$  to  $L$  and  $z_-(\mathbf{r})$  to 0. This transformation is easily implemented by

$$z' = \frac{Lz}{\Delta(\mathbf{r}) + L} - \frac{Lz_-(\mathbf{r})}{\Delta(\mathbf{r}) + L}, \quad \mathbf{r}' = \mathbf{r}, \quad (1)$$

where  $\Delta(\mathbf{r}) \equiv z_+(\mathbf{r}) - z_-(\mathbf{r}) - L$ . After transformation, the wavefunction can be generically expressed by  $\Psi_n = \psi_n(x, y) \sin\left(\frac{n\pi}{L}z'\right) / \sqrt{\frac{L+\Delta(\mathbf{r})}{2}}$  which satisfies the normalization condition:  $\int_0^{L+\Delta} dz \int d\mathbf{r} |\Psi_n|^2 = 1$ .

For typical quantum wells, the Fermi wavelength is about 400Å. If  $L$  is less than 340Å, there will be no band crossing at low temperatures, and we can take the average along  $z$  direction with respect to a given subband, i.e., average with respect to  $\sin\frac{n\pi}{L}z'$  ( $n$  will be taken to be one). In other words, the more appropriate Hamiltonian to work with is defined by

$$H_n = \langle \hat{H} \rangle \equiv \frac{\int_0^L dz' \sin\frac{n\pi}{L}z' \hat{H} \sin\frac{n\pi}{L}z'}{\int_0^L dz' \sin^2\frac{n\pi}{L}z'}. \quad (2)$$

After the averaging, we find that an extra potential  $\delta V$  is introduced to  $H_n = \frac{\hbar^2}{2m}\nabla^2 + \delta V$  where the Laplacian is over the  $(x, y)$  directions and

$$\begin{aligned} -\frac{2m}{\hbar^2}\delta V = & \alpha_n \frac{(\nabla A)^2}{A^2} + \beta_n \frac{2}{A} \nabla A \cdot (\nabla B - \frac{B}{A} \nabla A) \\ & + \gamma_n \left[ A^2 + \left( \nabla B - \frac{B}{A} \nabla A \right)^2 \right] + \delta_n \left( \frac{2}{A} \nabla A \cdot \nabla + \frac{1}{A} \nabla^2 A \right). \end{aligned} \quad (3)$$

Here  $A \equiv \frac{L}{\Delta(\mathbf{r})+L}$ ,  $B \equiv -\frac{Lz_-(\mathbf{r})}{\Delta(\mathbf{r})+L}$ ,  $\alpha_n \equiv \langle z'^2 \frac{\partial^2}{\partial z'^2} \rangle_n$ ,  $\beta_n \equiv \langle z' \frac{\partial^2}{\partial z'^2} \rangle_n$ ,  $\gamma_n \equiv \langle \frac{\partial^2}{\partial z'^2} \rangle_n$  and  $\delta_n \equiv \langle z' \frac{\partial}{\partial z'} \rangle_n$ . It is easy to show that  $\delta_n = -1/2$  is generally true.

If we expand  $\delta V$  to the linear order of  $\Delta/L$  and keep only up to  $O(z_-)$ , we obtain

$$\delta V = E_n - \frac{2E_n}{L}\Delta(\mathbf{r}) + \delta_n \frac{\hbar^2}{m} \left( \frac{1}{L} \nabla \Delta(\mathbf{r}) \cdot \nabla + \frac{1}{2L} \nabla^2 \Delta(\mathbf{r}) \right) - \beta_n \frac{\hbar^2 \nabla(z_+ - L) \cdot \nabla z_-}{mL}, \quad (4)$$

where we have identified  $-\gamma_n \hbar^2/2m$  as  $E_n$ . Note that the resulting Hamiltonian is invariant under reflection:  $L - z_- \rightarrow z_+$  and  $L - z_+ \rightarrow z_-$ . Let us first put the last term in the right place. For this purpose, we consider the two point correlation function of  $\Delta(\mathbf{r})$

$$\begin{aligned} \langle \Delta(\mathbf{r}) \Delta(\mathbf{r}') \rangle = & \langle (z_+(\mathbf{r}) - L)(z_+(\mathbf{r}') - L) \rangle + \langle z_-(\mathbf{r}) z_-(\mathbf{r}') \rangle \\ & - \langle (z_+(\mathbf{r}) - L) z_-(\mathbf{r}') \rangle - \langle (z_+(\mathbf{r}') - L) z_-(\mathbf{r}) \rangle. \end{aligned}$$

If the  $z_+(\mathbf{r})$  and  $z_-(\mathbf{r})$  are uncorrelated, the cross terms in the above equation vanish. In this case, if one assumes that the surfaces described by  $z_+(\mathbf{r})$  and  $z_-(\mathbf{r})$  are statistically the same, one obtains that  $\langle (z_+(\mathbf{r}) - L)(z_+(\mathbf{r}') - L) \rangle = \langle z_-(\mathbf{r})z_-(\mathbf{r}') \rangle = \langle \Delta(\mathbf{r})\Delta(\mathbf{r}') \rangle / 2$ . In other words, both  $z_+(\mathbf{r}) - L$  and  $z_-(\mathbf{r})$  are of the order of  $\Delta(\mathbf{r})$ . Therefore, the last term in Eq. (4) is of higher order and can be neglected. In addition to the special case when  $z_+(r) - L$  and  $z_-(r)$  are correlated, for instance, if either interface is smooth but tilted, i.e.,  $\nabla z$  is finite, this  $\nabla(z_+ - L) \cdot \nabla z_-$  term will also need to be considered.

In general, the second term in Eq.(4) has no definite relation with  $E_n$ . When  $L$  is the only length scale in the Hamiltonian (e.g., an infinite potential well),  $E_n$  has to be proportional to  $1/L^2$  and  $-\frac{2E_n}{L} = \frac{\partial E_n}{\partial L}$ . Eq.(4) can then be written as

$$\delta V = E_n + \frac{\partial E_n}{\partial L} \Delta(\mathbf{r}) - \frac{\hbar^2}{2m} \left[ \frac{1}{L} \nabla \Delta(\mathbf{r}) \cdot \nabla + \frac{1}{2L} \nabla^2 \Delta(\mathbf{r}) \right]. \quad (5)$$

Physically it becomes clear that the second term in Eq.(5) describes the local energy-level fluctuation, which was introduced phenomenologically in the literature for interface roughness scattering<sup>8,10</sup> but is now formally derived and shown to be valid only for an infinite potential well or any other potential with only one length scale. It is easy to check that, to the first order in ordinary perturbation theory, the third term in Eq.(5) does not contribute to the scattering matrix for single-particle states. However, as we shall derive in below, a closer investigation shows that this is not correct. Indeed, when this term is combined with the kinetic energy, it becomes

$$H' = -\frac{\hbar^2}{2m} \left( \nabla + \frac{\nabla \Delta(\mathbf{r})}{2L} \right)^2. \quad (6)$$

(a second order term has been neglected). Obviously, its effect is to modulate the wavefunction for every particle by

$$\Psi(\mathbf{r}) \rightarrow \Psi(\mathbf{r}) \exp\left(-\frac{\Delta(\mathbf{r})}{2L}\right). \quad (7)$$

Note that this result is *independent* of the depth of the well. There are two consequences: First, it causes fluctuations in the charge density. This is a many-particle effect and will

suppress the mobility. We will analyze it in the next section. Secondly, even for single-particle state, it implies that the transmission probability is not one when each particle passes by a step in the interface. When combined with the Landauer formula<sup>11</sup>, it indicates that the mobility will be further reduced. We will analyze this effect in the final section.

In summary, to the first order in  $\Delta(\mathbf{r})$ , the surface roughness introduces local energy level fluctuations and local wavefunction modulation for single particle states. Since the surface roughness modulates the single particle wavefunction in a coherent way, the wavefunction modulation does not introduce new scattering. In the single particle level, the effect of surface roughness is entirely contained in the local energy level fluctuations. We shall see in the next section that when we include many-particle interactions, the wavefunction modulation becomes as important as the energy level fluctuations.

### III. MANY-PARTICLE EFFECT

In this section, we discuss the many-particle effect that is due to the wavefunction modulation. We shall demonstrate its effect on the calculation of electron mobility. The change of the wavefunction induces a local modulation in the density of electrons:

$$n(\mathbf{r}, z') = n'(\mathbf{r}) \frac{\sin^2(\frac{n\pi}{L}z')}{(L + \Delta(\mathbf{r}))/2} \exp(-\frac{\Delta(\mathbf{r})}{L})$$

with the understanding that the normalization is done with respect to  $z$ . Here  $n'(\mathbf{r})$  is the 2-D electron density after being perturbed by the local energy level fluctuations,  $\frac{\partial E_n}{\partial L}\Delta(\mathbf{r})$ . It is easy to show that

$$n'(\mathbf{r}) = n_0 \left\{ 1 + \frac{2m}{\pi \hbar^2 k_F^2} \frac{\partial E_n}{\partial L} \int_{k \leq k_F} d^2\mathbf{k} \sum_{\mathbf{p}} \frac{[\Delta(\mathbf{k} - \mathbf{p}) \cdot e^{i(\mathbf{p}-\mathbf{k}) \cdot \mathbf{r}} + h.c.]}{k^2 - p^2} \right\}$$

where  $n_0 = k_F^2/2\pi$  is the equilibrium electron density at two dimensions and  $h.c.$  denotes a Hermitian conjugate of the previous term. We shall assume that the density of positive charge background remains unchanged so that the local charge modulation is entirely due to electrons. The change of charge density is

$$\delta\rho(\mathbf{r}, z) = en(\mathbf{r}, z')\theta(z - z_-)\theta(L + \Delta - z) - en_0 \frac{\sin^2\left(\frac{n\pi}{L}z\right)}{L/2} \theta(z) \theta(L - z). \quad (8)$$

For convenience, we shall assume  $z_- = 0$  and neglect the curvature effect due to the roughness (for instance, the special case when both interfaces fluctuate while their spacing remains  $L$ ).

To the first order in  $\Delta(\mathbf{r})$ , the total electric potential  $\delta\phi$  satisfies

$$\begin{aligned} -(\nabla^2 + \frac{\partial^2}{\partial z^2})\delta\phi(\mathbf{r}, z) = 4\pi\rho_{ind} + 4\pi en_0 \frac{\sin^2(\frac{n\pi}{L}z)}{L/2} \left\{ -2 \left[ 1 + \frac{n\pi z}{L} \cot\left(\frac{n\pi}{L}z\right) \right] \frac{\Delta(\mathbf{r})}{L} \right. \\ \left. + \frac{m}{\pi^2 \hbar^2 n_0} \frac{\partial E_n}{\partial L} \int_{k \leq k_F} d^2\mathbf{k} \sum_{\mathbf{p}} \frac{[\Delta(\mathbf{k} - \mathbf{p}) \cdot e^{i(\mathbf{p} - \mathbf{k}) \cdot \mathbf{r}} + h.c.]}{k^2 - p^2} \right\} \theta(z)\theta(L - z), \quad (9) \end{aligned}$$

where  $\rho_{ind}$  is the induced charge density. The associated scattering matrix within a given subband is given by

$$\begin{aligned} \delta M(\mathbf{q}) &= \langle \mathbf{k} | \delta V | \mathbf{q} - \mathbf{k} \rangle_n \\ &= \int d^2\mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} \frac{\int_0^L dz \delta V(\mathbf{r}, z) \sin^2(\frac{n\pi}{L}z)}{L/2} \\ &= \frac{2e}{L} \int_0^L dz \delta\phi(\mathbf{q}, z) \sin^2(\frac{n\pi}{L}z), \quad (10) \end{aligned}$$

where  $\delta\phi(\mathbf{q}, z)$  is of the order of  $\Delta$ . We shall denote  $\int_0^L dz \delta\phi(\mathbf{q}, z) \sin^2(\frac{n\pi}{L}z)$  by  $\delta\tilde{\phi}(\mathbf{q})$ .

We now express the induced charge density in terms of  $\delta\tilde{\phi}(\mathbf{q})$ . This can be achieved in the conventional linear response theory by

$$\rho_{ind}(\mathbf{q}, \omega = 0, z) = \int dz' \text{Re} \Pi(q, \omega = 0, z, z') e^2 \delta\phi(\mathbf{q}, z'), \quad (11)$$

where  $\Pi(q, \omega = 0, z, z')$  is the polarization insertion<sup>13</sup>. If we focus on the  $n$ -th subband, the one-loop contribution to  $\Pi(q, \omega = 0, z, z')$  is

$$\text{Re} \Pi(q, \omega = 0, z, z') = \sin^2(\frac{n\pi}{L}z) \sin^2(\frac{n\pi}{L}z') \frac{-16m}{\hbar^2 L^2} \mathcal{P} \int \frac{d^2k}{(2\pi)^2} \theta(1 - k) \frac{1}{qk(\cos\theta + x)}, \quad (12)$$

where  $q$  and  $k$  are measured in terms of  $k_F$ ,  $\theta(1 - k)$  is the step function,  $x \equiv q/2k$ , and  $\mathcal{P}$  denotes the Cauchy principle value. It is easy to show that

$$\mathcal{P} \int_0^{2\pi} d\theta \frac{1}{\cos\theta + x} = \begin{cases} 0 & \text{if } |x| < 1 \\ \frac{2\pi}{\sqrt{x^2 - 1}} & \text{if } |x| \geq 1 \end{cases} \quad (13)$$

Since the momentum transfer  $q$  is always less than  $2k_F$ ,  $x < 1$  for the range of  $k$  integration.

We find that

$$\mathcal{P} \int \frac{d^2k}{(2\pi)^2} \theta(1-k) \frac{1}{qk(\cos\theta + x)} = \int_0^{q/2} \frac{dk}{2\pi} \frac{1}{q\sqrt{(q/2k)^2 - 1}} = \frac{1}{4\pi}. \quad (14)$$

As a result, we obtain

$$\rho_{ind}(\mathbf{q}, \omega = 0, z) = -\frac{4me^2}{L^2\pi\hbar^2} \sin^2\left(\frac{n\pi}{L}z\right) \delta\tilde{\phi}(\mathbf{q}). \quad (15)$$

Substituting the above into Eq.(9) and performing Fourier transformation on both  $\mathbf{r}$  and  $z$ , we find

$$\begin{aligned} (q^2 + k_z^2) \delta\phi(\mathbf{q}, k_z) = & -\frac{16me^2}{L^2\hbar^2} v(k_z) \delta\tilde{\phi}(\mathbf{q}) - \frac{16\pi en_0}{L^2} \Delta(\mathbf{q}) [u(k_z) + v(k_z)] \\ & + \frac{16me}{\pi L\hbar^2} \frac{\partial E_n}{\partial L} \int_{k \leq k_F} d^2\mathbf{k} \frac{\Delta(\mathbf{q})}{k^2 - |\mathbf{k} - \mathbf{q}|^2} v(k_z), \end{aligned} \quad (16)$$

where  $u(k_z) = \frac{n\pi}{2L} \int_0^L e^{ik_z z} z \sin\left(\frac{2n\pi}{L}z\right) dz$  and  $v(k_z) = \int_0^L e^{ik_z z} \sin^2\left(\frac{n\pi}{L}z\right) dz$ . The  $\mathbf{k}$  integration has been done in Eq.(14). It is also easy to show that

$$\delta\tilde{\phi}(\mathbf{q}) = \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \delta\phi(\mathbf{q}, k_z) v^*(k_z) \quad (17)$$

Substituting  $\delta\phi(\mathbf{q}, k_z)$  in the above equation, we obtain

$$\begin{aligned} \delta\tilde{\phi}(\mathbf{q}) = & -\int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \frac{|v(k_z)|^2}{q^2 + k_z^2} \left[ \frac{16\pi en_0}{L^2} \Delta(\mathbf{q}) + \frac{16me^2}{L^2\hbar^2} \delta\tilde{\phi}(\mathbf{q}) - \frac{8me}{L\hbar^2} \frac{\partial E_n}{\partial L} \Delta(\mathbf{q}) \right] \\ & - \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \frac{v^*(k_z) \cdot u(k_z)}{q^2 + k_z^2} \frac{16\pi en_0}{L^2} \Delta(\mathbf{q}). \end{aligned} \quad (18)$$

The  $k_z$  integration can be analytically solved as:

$$I(q) \equiv \int \frac{dk_z}{2\pi} \frac{|v(k_z)|^2}{q^2 + k_z^2} = \frac{L}{2} \left[ \frac{1}{q^2} + \frac{1}{2[q^2 + (2n\pi/L)^2]} \right] + \frac{(2n\pi/L)^4}{4q^3} \frac{e^{-qL} - 1}{[q^2 + (2n\pi/L)^2]^2} \quad (19)$$

$$\begin{aligned} J(q) & \equiv \int \frac{dk_z}{2\pi} \frac{v^* u}{q^2 + k_z^2} \\ & = \left(\frac{n\pi}{L}\right)^3 \left[ \frac{4}{qL} \frac{e^{-qL} - 1}{[q^2 + (2n\pi/L)^2]^3} + \frac{n\pi e^{-qL}}{q^2 [q^2 + (2n\pi/L)^2]^2} - \frac{n\pi}{q^2} \left(\frac{L}{2n\pi}\right)^4 \right]. \end{aligned} \quad (20)$$

With a little rearrangement, Eq.(18) gives



$$\delta\tilde{\phi}(\mathbf{q}) = \frac{\frac{16\pi en_0}{L^2} [I(q) + J(q)] - \frac{8m\epsilon}{L\hbar^2} \frac{\partial E_n}{\partial L} I(q)}{1 + \frac{16me^2}{L^2\hbar^2} I(q)} [-\Delta(\mathbf{q})] \quad (21)$$

For a narrow quantum well satisfying  $qL \leq 2k_F L \ll 1$  (this requires  $L \ll 33\text{\AA}$  for  $n_0 \approx 2 \times 10^{15} \text{m}^{-2}$  in quantum wells),  $I(q) \approx \frac{L^2}{8q}$  and  $J(q) \approx -\frac{L^2}{16q}$  and Eq.(21) reduces to the standard 2D screening form<sup>9</sup>:

$$\delta\tilde{\phi}(\mathbf{q}) = \frac{\alpha}{q + q_s} [-\Delta(\mathbf{q})] \quad (22)$$

(the second term in the denominator of Eq.(21) does not exist in pure two dimensions) where  $q_s = 2me^2/\hbar^2 \simeq 1/(0.25 \text{\AA})$  and  $\alpha = \pi en_0$ .

However, if  $qL \approx 1$ , one shall have to use the full expression of  $I(q)$  and  $J(q)$ . Since  $\frac{16me^2}{L^2\hbar^2} \simeq 10^{30} \text{m}^{-3}$  and  $I(q) \simeq 10^{-27} \text{m}^3$ , the second term in the denominator of Eq.(21) dominates and  $\delta\tilde{\phi}(\mathbf{q}) \approx \frac{\pi n_0 \hbar^2}{2em} \Delta(\mathbf{q})$ . The resulting scattering matrix within a given subband is thus given by

$$\begin{aligned} |M(\mathbf{q})|^2 &= \langle |\delta V(\mathbf{q})|^2 \rangle = \frac{1}{\aleph} \left( \frac{\partial E_n}{\partial L} - \frac{\frac{32\pi e^2 n_0}{L^3} [I(q) + J(q)] - \frac{16me^2}{L^2\hbar^2} \frac{\partial E_n}{\partial L} I(q)}{1 + \frac{16me^2}{L^2\hbar^2} I(q)} \right)^2 S(q) \\ &\approx \frac{1}{\aleph} \left( 2 \frac{\partial E_n}{\partial L} - \frac{2n_0 \pi \hbar^2}{mL} \right)^2 S(q), \end{aligned} \quad (23)$$

where  $\aleph$  is the normalization and  $S(q)$  is the power spectrum of  $\Delta(\mathbf{q})$ , given<sup>10</sup> by  $\langle |\Delta(\mathbf{q})|^2 \rangle$ .

Given the scattering matrix, we can calculate the relaxation time via the relation

$$\frac{1}{\tau(\mathbf{k})} = \frac{1}{2\pi\hbar} \int d^2k' |M(\mathbf{k} - \mathbf{k}')|^2 (1 - \cos \Phi) \delta(E(\mathbf{k}) - E(\mathbf{k}')), \quad (24)$$

where  $\Phi$  denotes the angle between the initial and final wavevectors  $\mathbf{k}$  and  $\mathbf{k}'$ . The mobility of the electron can then be solved by

$$\mu = e \int dE \frac{\rho(E) v_x^2(E) \tau(E)}{4n k_B T \cosh^2((E - E_F)/2k_B T)}. \quad (25)$$

We see that the interparticle interaction reduces the electron mobility estimated by the energy level fluctuations by at least three quarters. Since  $\frac{\partial E_n}{\partial L} < 0$ , the second term in Eq.(23) due to wavefunction modulation increases the scattering matrix and further reduces

the mobility. The overall reduction of the mobility in comparison to previous approach is about 1/4.

We note in passing that in general, in addition to the above Coulomb interaction, the density modulation induced by the surface roughness also affects any interactions that depend on the electron density. If in the absence of surface roughness, the interaction is described by  $\int d\mathbf{r} \int d\mathbf{r}' \hat{n}(\mathbf{r}) V_0(\mathbf{r}, \mathbf{r}') \hat{n}(\mathbf{r}')$ , then formally the effect of surface roughness can be simply included by replacing  $V_0$  by

$$V(\mathbf{r}, \mathbf{r}') \approx V_0(\mathbf{r}, \mathbf{r}') \left( 1 - \frac{\Delta(\mathbf{r}) + \Delta(\mathbf{r}')}{L} \right). \quad (26)$$

#### IV. DISCUSSIONS AND CONCLUSIONS

In this section, we examine the validity of our approach by studying a simplified rough interface:  $z_+ = L \cdot \theta(-x) + (L + \Delta) \cdot \theta(x)$  and  $z_- = 0$ , i.e., a step at  $x = 0$  (see Fig. 2). We shall directly investigate the solution without using the effective Hamiltonian Eq.(3) and show that they are consistent with each other. Let us first fix the boundary condition by requiring the wavefunction to be travelling waves when far from the step: i.e.,  $\Psi(x, z) \rightarrow (e^{ikx} + \mathcal{R}e^{-ikx}) \sin(\pi z/L)$  as  $x \rightarrow -\infty$  and  $\Psi(x, z) \rightarrow \mathcal{T}e^{ipx} \sin(\pi z/(L + \Delta))$  as  $x \rightarrow \infty$ . When we approach  $x = 0$ , higher subbands begin to participate, and the most general form for the wavefunction is

$$\Psi(x, z) = \begin{cases} (e^{ikx} + \mathcal{R}e^{-ikx}) \sin \frac{\pi z}{L} + \sum_{n=2}^{\infty} b_n e^{k_n x} \sin \frac{n\pi z}{L}, & \text{for } x \geq 0 \\ \mathcal{T}e^{ipx} \sin \frac{\pi z}{L+\Delta} + \sum_{l=2}^{\infty} a_l e^{-p_l x} \sin \frac{l\pi z}{L+\Delta}, & \text{for } x < 0 \end{cases} \quad (27)$$

where  $k_n$  and  $p_l$  are positive and satisfy the energy conservation condition:

$$-k_n^2 + \left( \frac{n\pi}{L} \right)^2 = -p_l^2 + \left( \frac{l\pi}{L+\Delta} \right)^2 = k^2 + \left( \frac{\pi}{L} \right)^2 = p^2 + \left( \frac{\pi}{L+\Delta} \right)^2. \quad (28)$$

The fact that  $\pi/L$  is comparable to the Fermi momentum makes these higher subbands (with  $n, l$  greater than one) correspond to decaying modes when  $\Delta \ll L$ . Also in this limit,

since  $\mathcal{R}$ ,  $b_n$  and  $a_l$  vanish when  $\Delta = 0$ , we expect them to be no greater than the order of  $O(\Delta/L)$ .

To find the coefficients in  $\Psi(x, z)$ , we apply the matching conditions at  $x = 0$

$$\Psi(0^+, z) = \begin{cases} \Psi(0^-, z), & \text{for } 0 \leq z \leq L \\ 0, & \text{for } L \leq z \leq L + \Delta \end{cases} \quad (29)$$

$$\partial_x \Psi(0^+, z) = \partial_x \Psi(0^-, z) \text{ for } 0 \leq z \leq L. \quad (30)$$

By using the completeness relation of  $\sin(\pi z/(L + \Delta))$  and Eq.(29), we obtain

$$a_l = (1 + \mathcal{R})Y(1, l) + \sum_{n=2}^{\infty} b_n Y(n, l), \quad (31)$$

where  $a_1 \equiv \mathcal{T}$  and  $Y(n, l)$  is defined by

$$\begin{aligned} Y(n, l) &\equiv \frac{2}{L + \Delta} \int_0^L dz \sin \frac{n\pi z}{L} \sin \frac{l\pi z}{L + \Delta} \\ &= \frac{2n(-1)^n}{L(L + \Delta)\pi} \frac{\sin \frac{\ell\pi L}{L + \Delta}}{\left(\frac{\ell}{L + \Delta}\right)^2 - \left(\frac{n}{L}\right)^2}. \end{aligned} \quad (32)$$

This implies that  $Y(n, l) = O(\Delta/L)$  when  $n \neq l$ , while  $Y(n, l) = O(1)$  when  $n = l$ . This fact, when combined with Eq.(31), yields

$$\mathcal{T} = (1 + \mathcal{R})Y(1, 1) + O(\Delta^2/L^2). \quad (33)$$

Similarly, using the completeness relation of  $\sin(\pi z/L)$  and Eq.(30), we obtain

$$ik(1 - \mathcal{R}) = \frac{L + \Delta}{L} \left( ip\mathcal{T}Y(1, 1) - \sum_{l=2}^{\infty} a_l p_l Y(1, l) \right), \quad (34)$$

which, to first order in  $\Delta/L$ , reduces to

$$k(1 - \mathcal{R}) = \frac{L + \Delta}{L} p\mathcal{T}Y(1, 1) + O(\Delta^2/L^2). \quad (35)$$

By combining Eqs.(33) and (35), the coefficient  $\mathcal{T}$  can be determined as  $-\frac{\Delta}{2L} \left(1 + \frac{\pi^2}{k^2 L^2}\right)$ . Note that the second term  $-\frac{\Delta}{2L}$  reproduces precisely the rescaling of wavefunction in Eq.(7), while the third term  $-\frac{\Delta\pi^2}{2k^2 L^3}$  is nothing but the same reduction<sup>14</sup> of transmitted amplitude in the 1-D Schrodinger equation with a potential barrier of height,  $\frac{\partial E}{\partial L} \Delta$  (the energy level fluctuations in Eq.(5)):

$$\mathcal{T} = \frac{2}{1 + \sqrt{1 + (2\pi^2\Delta/k^2L^3)}} \simeq 1 - \frac{\Delta\pi^2}{2k^2L^3}. \quad (36)$$

Although  $\Delta$  is assumed to be positive in the above derivations, we have checked that our conclusions remains valid when  $\Delta$  is negative.

We have thus seen that the validity of our effective Hamiltonian approach has been fully checked. We now briefly re-examine the effect due to the change of the single-particle state in the ballistic regime. For a single step as we considered in the above, according to the Landauer formula<sup>11</sup>, the conductance due to the step is given by

$$G = \frac{e^2}{\pi\hbar} \frac{T}{R}, \quad (37)$$

where  $T$  and  $R$  are transmission and reflection probability. A simple analysis shows that the mobility is given by

$$\mu = \frac{|e|\hbar}{\pi\hbar n_0} \frac{T}{R} \simeq \frac{|e|\hbar}{\pi\hbar n_0} \left[ \frac{L(1 + \pi^2/k_F^2 L^2)}{\Delta} - 1 \right] \simeq 4836 \left[ \frac{L(1 + \pi^2/k_F^2 L^2)}{\Delta} - 1 \right] \frac{\text{cm}^2}{\text{V sec}} \quad (38)$$

When the system has many steps, we simply replace  $\Delta$  by  $\sum \Delta_i$ . Since  $\Delta$  is at the order of 3-4 Å, we can estimate  $\sum \Delta_i$  by the same order. Therefore,  $\mu$  is about  $10^4 - 10^5 \text{cm}^2/\text{V sec}$  for  $L = 100 \text{ Å}$ . This number when combined with the contribution from Eq.(23) ( $\sim 10^5 \text{cm}^2/\text{V sec}$ ) predicts that the mobility is at the order of  $10^4 \text{cm}^2/\text{V sec}$ , in close to experimental result<sup>15</sup>.

In conclusion, we have derived an effective Hamiltonian for two dimensional quantum wells with rough interfaces. It is checked to give consistent results for an exactly solvable model. Two new terms are generated. The first term is identified to the local energy level fluctuations, which was introduced phenomenologically in the literature but the previous form is now shown to be valid only when the Hamiltonian has one single length scale. The effect of this term on the electron mobility has been discussed before. The other term is a new finding, which is shown to modulate the wavefunction and cause fluctuations in the charge density. We discuss its effects on the reduction of the electron mobility both at the level of the single-particle state and by including the many-particle interactions. An estimate of the electron mobility is made and gives rises to correct order in comparison to experimental data.

## **V. ACKNOWLEDGMENTS**

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<sup>(a)</sup> E-mail: mou@phys.nthu.edu.tw

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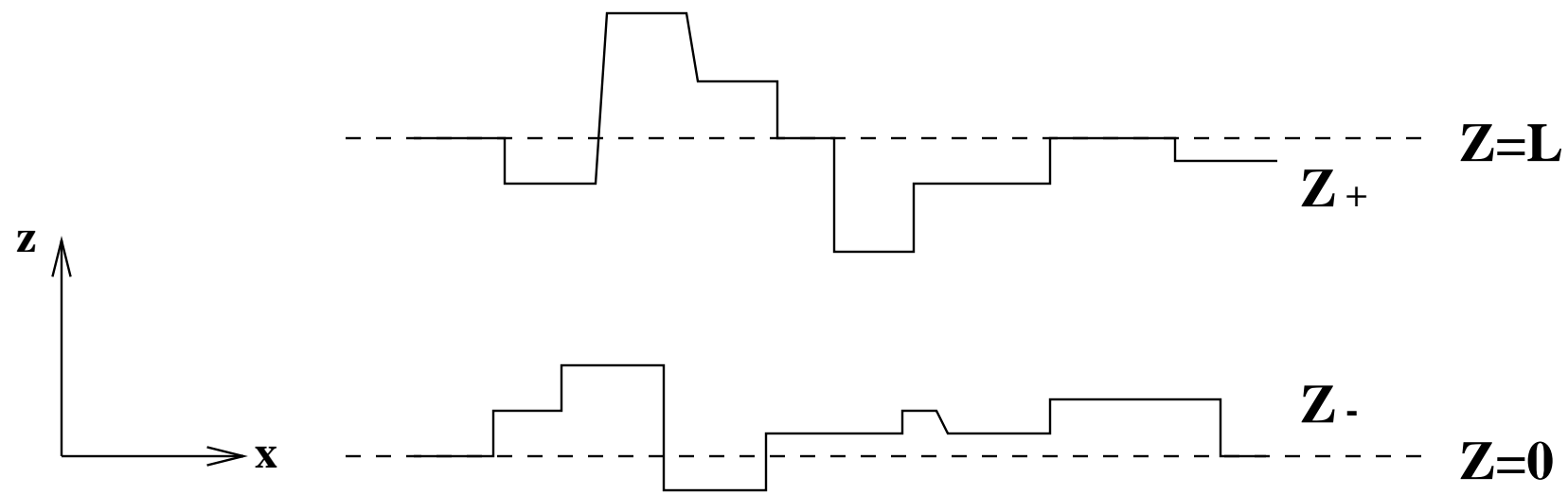
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### **Figure Captions:**

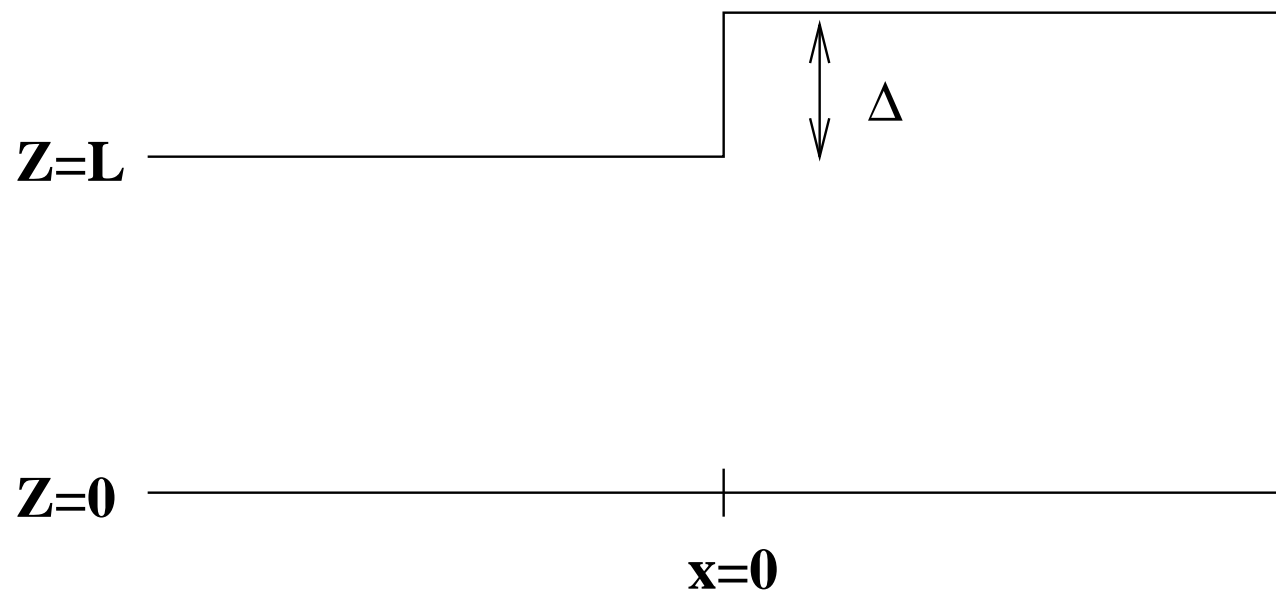
**Fig. 1** A schematic plot of a 2D quantum well with rough interfaces

**Fig. 2** A simple step at  $x = 0$  can be solved asymptotically.



**Fig. 1**





**Fig. 2**